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Time reversal symmetry breaking superconducting states in Cuprates

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Abstract : We study the doping and temperature dependence of the order parameter for the time reversal symmetry breaking states $d_{x^2-y^2}$ + *is* and $d_{x^2-y^2} + id_{xy}$ using a tight binding model that includes orthorhombic distortion and second nearest neighbor hopping, γ. Mixing occurs both in square lattice and in the presence of orthorhombic distortion and also for various values of γ when studied as a function of filling. We also study the specific heat for the mixed states and the coherence length for the pure $d_{x^2-y^2}$ and d_{xy} waves.

Keywords : Order parameter, symmetry breaking, super conducting, cuprates.

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n 1986 superconductivity was discovered in LBCO (an xide of Lanthanum, Barium and Coper) with critical emperature $T_c \approx 35$ K initiating the era of high temperature uperconductors (HTSC) [1]. In these 13 years the critical emperature has increased considerably to reach nearly four mes the limit considered in the conventional superconductors nd the most promising ones are those containing an oxide f copper, known as cuprates. The cuprates consist of one r more CuO_2 planes in their structure separated by layers f other atoms (Ba, La...). Presently two of the leading andidates for technological application of superconductivity re $LnBa_2Cu_3O_{7-\delta}$ and $Bi_2Sr_2Ca_2Cu_3O_{10}$. Most of the cuprates re doped materials. For example, substitution of the divalent r for La in the antiferromagnetic insulator La_2CuO_4 produces uperconductivity in $La_{2-x}Sr_xCuO_4$ [2]. T_c is also very ensitive to the level of doping. These new materials not only how a high T_c but also various anomalous normal state roperties. The peculiarities of these superconductors have een a challenge for the thousands of scientists working round the globe.

The pairing symmetry provides clue to the identity of the uperconducting pairing mechanism which is essential for development of the theory of HTSC. It still remains a ubject of intense debate even after more than a decade of intense research [3]. Unlike the conventional superconductors these new materials are not *s*-wave compounds. Several experiments and theoretical studies suggest a $d_{x^2-y^2}$ wave pairing in cuprates. The phase sensitive pairing symmetry experiments [4] have given a strong evidence for predominantly anisotropic *d*-wave pairing in a number of optimally doped cuprates. However, there have also been considerable theoretical studies [5,6] indicating that a pure $d_{x^2-y^2}$ is not stable against the formation of time reversal symmetry breaking states such as $d_{x^2-y^2} + id_{xy}$ or $d_{x^2-y^2}$ + *is* below a certain characteristic temperature. Various indirect experimental evidences for the existence of a major *d*-wave component with a minor imaginary *s* and d_{xy} component have been reported in cuprates like $YBa_2Cu_3O_7$ [7] and $Bi_2Sr_2CaCu_2O_8$ [6] respectively.

Till today there has been no consensus as to the mechanism causing high T_c in these materials. So the search for the new materials has been empirical as no predictive theory is currently known. In absence of a microscopic theory we use a phenomenological two-dimensional tight binding model with appropriate lattice symmetry.

We study the two-dimensional single-band tight binding model with electronic dispersion relation including upto second nearest neighbor hopping to investigate the behavior of the states $d_{x^2-y^2}+i\chi$ with filling and temperature. Here χ can be s or d_{xy}. We consider the order parameter dependence on filling and temperature both in square lattice and also in presence of orthorhombic distortion. We also exhibit the temperature dependence of specific heat for the ' .c wave and the coherence length of the pure d waves. The quasiparticle dispersion relation is given by $\varepsilon_k=-2t[\cos k_x+\beta\cos k_y\;-\gamma\cos k_x\cos k_y-\mu]$, where t and βt are the nearest neighbor hopping integrals along the in plane a and b axes respectively and γt is the second nearest neighbor hopping integral. μ is the chemical potential. The gap (Δ_k) equation in this model is

$$\Delta_k=-\sum_q V_{kq}\frac{\Delta_q}{2E_q}\tanh\frac{E_q}{2k_BT}, \tag{1}$$

with $E_q=\left[(\varepsilon_q-E_F)^2+|\Delta_q|^2\right]^{1/2}$, where E_F is the Fermi energy and k_B is the Boltzmann constant. The interaction is given by $V_{kq}=-\sum_i V_i\eta_{ik}\eta_{iq}$ irreducible representation of the point group of square lattice C_{4v} and are appropriate generalization of the circular harmonics incorporating the proper lattice symmetry. We define $\eta_{1k}=\cos k_x-\beta\cos k_y$, for $d_{x^2-y^2}$ wave, and $\eta_{2k}=2\sin k_x\sin k_y$ (1) for $d_{xy}(s)$ wave. The order parameter has the following anisotropic form : $\Delta_k\equiv\Delta_1(\cos q_x-\beta\cos q_y)+i\Delta_2\eta_{2k}$ where η_{2k} can be for s or d_{xy} wave. Using the above forms of Δ_q and V_{kq}, eq. (1) becomes a coupled set of equations, where the coupling is introduced through E_q [8,9,10]. The filling dependence can be determined from the number equation

$$n=1-\sum_q\frac{\varepsilon_q-\mu}{E_q}\tanh\frac{E_q}{2k_BT}. \tag{2}$$

We also study the specific heat $C_s(T)$ and coherence length ξ^2.

We solve the coupled set of gap equations [8,9] along with (2) numerically and calculate Δ_1 and Δ_2 at various n and temperatures. We perform calculations on a perfect square lattice ($\beta=1$) for both $d_{x^2-y^2}+i\chi$ mixing with $V_1=1.7t$, and $V_2=0.73t$. In the presence of an orthorhombic distortion ($\beta=.95$) the potentials are $V_1=2.1t$, and $V_2=0.97t$.

In Figure 1 we plot $\Delta_{x^2-y^2}=\Delta_1$ and $\Delta_{xy}=\Delta_2$ for $d_{x^2-y^2}+id_{xy}$ with $\gamma=0$ and 0.1. Mixing is present in all the above cases with $d_{x^2-y^2}$ as the dominant component. As n decreases we observe a rapid fall of the $d_{x^2-y^2}$ wave leading only to the d_{xy} wave. We observe a pronounced maximum in the $d_{x^2-y^2}$ wave accompanied by a minimum in the d_{xy} wave. Moreover, the maximum shifts towards a lower value of n as we increase γ. Unlike the $\beta=1$ case, we observe a dip near the maximum along with a rise in the minimum for $\beta=.95$ case.

In Figure 2 we plot Δ_1 and $\Delta=\Delta_2$ in case of $d_{x^2-y^2}+$ wave for the same parameters as in Figure 1 [9]. We observ similar behavior as in the previous case, except that t variation is much sharper. d_{xy} wave falls faster than s wa with n and goes to zero much earlier.

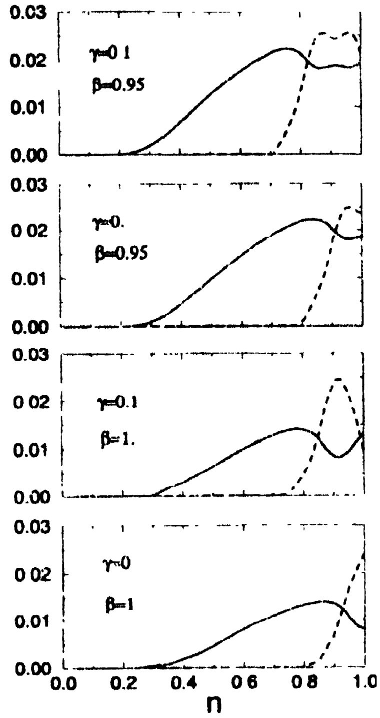

Figure 1. The order parameters $\Delta_{x^2-y^2}$ (dashed line), Δ_{xy} (full line) $(d_{x^2-y^2}+id_{xy})$-wave at different filling.

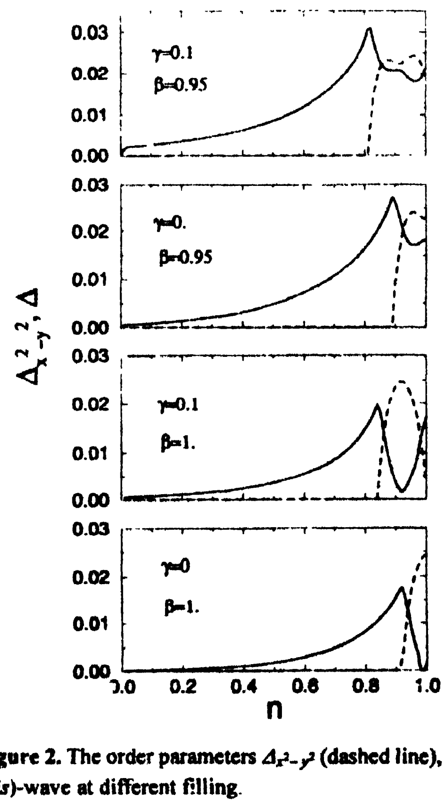

Figure 2. The order parameters $\Delta_{x^2-y^2}$ (dashed line), Δ (full line) for $(d_{x^2-y^2}$ $+\,is)$-wave at different filling.

In Figure 3 we plot the temperature dependence of the specific heat for the normal state and for $d_{x^2-y^2} + is$ states for μ , $V_2 = .73t$ and two values of V_0 : *i*) $V_0 = 1.92t$ and ii) $V_0 = 1.8t$. The specific heat shows two jumps one at T_c and the other at T_{c1} ($\Delta_2 = 0$). Hence we observe a second phase transition at T_{c1} [8,9,11]. For $T < T_{c1}$ the temperature dependence of the mixed wave specific heat is exponential s-wave type. Above T_c the curve follows the power-law behavior of the pure $d_{x^2-y^2}$. In $d_{x^2-y^2} + id_{xy}$ state we observe similar behavior [8].

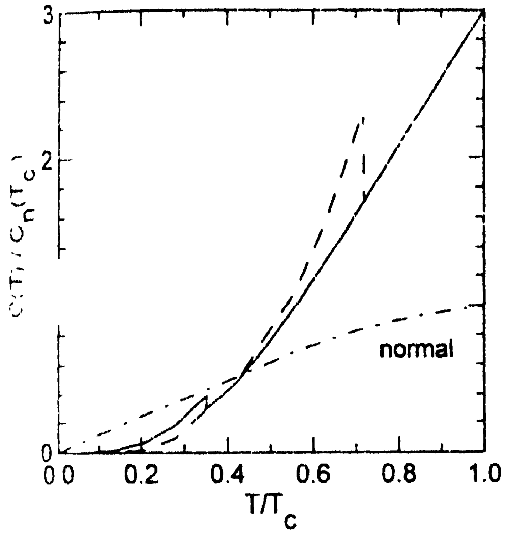

Figure 3. Specific heat ratio $C(T)/C_n(T_c)$ vs T/T_c for ($d_{x^2-y^2} + is$) for models (i) (dashed line) (ii) (full line) and the normal state (dashed-dotted line)

In Figures 4 and 5 we plot the coherence length as a function of filling for pure $d_{x^2-y^2}$ and d_{xy} states. For higher values of n, ξ^2 approximately remains constant but for high doping we find a steady increase in its value [12].

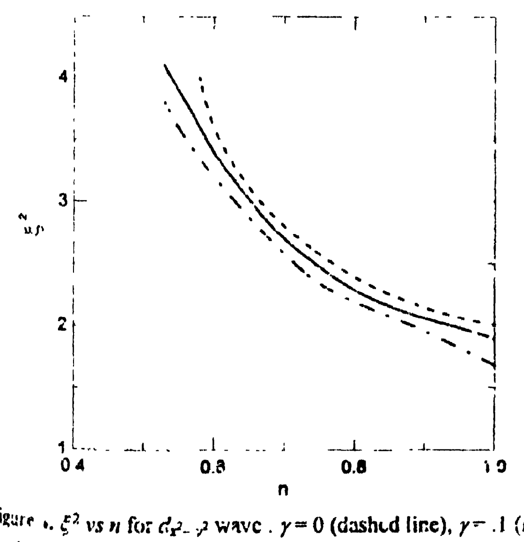

Figure 4. ξ^2 vs n for $d_{x^2-y^2}$ wave . $\gamma = 0$ (dashed line), $\gamma = .1$ (full line) and $\gamma = .2$ (dashed-dotted line).

We also observe a decrease in the value of ξ with a increase in γ for constant n. It is also in accord with the experimental values.

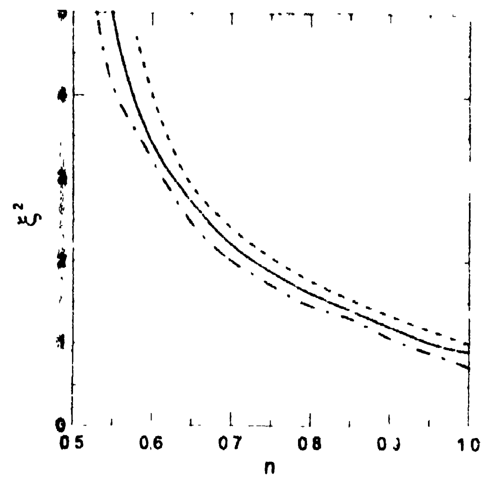

Figure 5. ξ^2 vs n for d_{xy} wave $\gamma = 0$ (dashed line), $\gamma = .1$ (full line) and $\gamma = .2$ (dashed-dotted line)

In conclusion, we have studied the ($d_{x^2-y^2} + i\chi$)-wave superconductivity employing a two-dimensional tight binding model on square lattice and also for orthorhombic distortion. We observe that both d_{xy} and s wave mix with the $d_{x^2-y^2}$ wave in square lattice and that with orthorhombic distortion indepenedent of the value of γ. At low doping we have the system is mainly dominated by $d_{x^2-y^2}$ wave. We also observe a second phase transition at T_{c1} from Figure 3. We thank FAPESP for financial support.

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